

IN THE SPECIFICATION

Please replace the title with the following title:

-- METHODS OF USING THE STRUCTURE COORDINATES OF
MOLECULES COMPRISING AN IMPDH-LIKE BINDING POCKET --

Please add the following paragraph as the first sentence of the specification
directly following the title:

B1 -- This application is a divisional of United States Application
08/640,164, filed April 30, 1996, now United States Patent 6,128,582. --

IN THE CLAIMS

Please cancel claims 24-25.

Please amend claim 23 and 36 as follows:

subcl
B2 23. (Twice Amended) A method for evaluating the ability of a chemical
entity to associate with a molecule or molecular complex comprising all or any part of a
binding pocket defined by structure coordinates of Chinese hamster type II inosine
monophosphate dehydrogenase ("IMPDH") amino acids 68, 69, 93, 273, 274, 275, 276,
277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413,
414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1, or a homologue
of said molecule or molecular complex, wherein said homologue comprises a binding
pocket that has a root mean square deviation from the backbone atoms of said amino acids
of not more than 1.5 Å, comprising the steps of:

BP C1
C1
a) employing computational means, which utilize said structure coordinates, to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex;

b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket; and

c) outputting said quantified association to a suitable output hardware.

B3 C2
29. (Amended) A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means, which utilize said structure coordinates, to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex;

b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket; and